M.Sc., CHEMISTRY – PROGRAMME STRUCTURE

I YEAR – I SEMESTER
COURSE CODE: 7MCH1C1

CORE COURSE-I–ORGANIC CHEMISTRY–I

Objectives:

- To impart a knowledge of Electron Displacement.
- To be familiar with the details of Stereochemistry, Aromaticity and detailed study of aliphatic nucleophilic substitution.

Unit I: Electron Displacement [15 hrs]

Inductive and Field Effects – Bond Distance – Bond Energies – Delocalized Bonds – Cross Conjugation – Steric Inhibition of Resonance – Hyper Conjugation – Effects of Structure on the Dissociation Constants of Acids and Bases.

Quantitative Treatment of the Effect of Structure on Reactivity – The Hammett Relationship – Significance of Reaction and Substituent Constants – Application of the Hammett Equation in Reaction Mechanism – Limitations, Modification and Deviations – Taft Equation.

Unit II: Stereochemistry [15 hrs]

Symmetry Elements and Point Group Classification – Conditions for Optical Activity – Optical Isomerism – Definitions – Newmann, Sawhorse and Fisher Projection Formulae – Concept of Chirality – The Cahn-Ingold-Prelog System of Nomenclature – Enantiotopic and Diastereotopic Atoms, Groups and Faces – Molecules with more than One Chiral Centre – Molecular Dissymmetry – Optical Activity of Biphenyls, Allenes and Spirans – Optical Isomerism of Nitrogen and Sulphur Compounds – Asymmetric Synthesis – Cram's Rule.

Geometrical Isomerism:

E-Z Nomenclature – Determination of Configuration of Geometrical Isomers Using Physical and Chemical Methods.

Unit III: Aromaticity [15 hrs]

Aromatic Character in Benzene, Six – Membered Rings, Five, Seven and Eight Membered Rings – Huckel's Rule and Craig's Rule – Concept of Homoaromaticity and Antiaromaticity – Systems with 2, 4, 8 and 10π Electrons – Systems with more than 10π Electrons – Alternant and Nonalternant Hydrocarbons. Chemistry of Cyclopentadienyl Anion – Fulvene – Azulene –Sydnones. (12), (14), (16), (18) – annulenes. Nomenclature of Bicyclic Systems.

Unit IV: Introduction to Reaction Mechanism [15 hrs]

Reactive Intermediates – Free radicals – Carbenes – Carbanions – Carbocations – Formation and Stability of Reactive Intermediates – Principle of Microscopic Reversibility – Hammond Postulate.

Aromatic Electrophilic Substitution – Orientation – Reactivity – Mechanism of Nitration, Friedel – Craft's Reaction – Ortho/Para Ratio

Aromatic Nucleophilic Substitution Reactions – S_NAr, S_N1 and Benzyne Mechanisms.

Unit V: Aliphatic Nucleophilic Substitution and Elimination [15 hrs]

Aliphatic Nucleophilic Substitution: Nucleophilicity and basicity – S_N^1 and S_N^2 mechanism – Effect of substrate structure – effect of reaction medium – effect of leaving group – ambident nucleophile – ambident substrates – symphoria – Neighbouring group participation of n, π and σ electrons – S_N^i mechanism – Nucleophilic substitution at allylic carbon and vinyl carbon

Elimination: α – elimination, β – elimination – E1, E2 and E1CB mechanism – stereo chemistry of elimination – orientation of double bond – Pyrolytic cis elimination – Bredt's rule.

Books for Reference:

1. Finar I.L., Organic Chemistry, Vol. II, 5th Edition, ELBS, England, 1975.
2. Morrison R.T., and Boyd R.N., Organic Chemistry, Prentice–Hall, 6th Edition, New Delhi, 1995.
3. Ferguson L.N., The Modern Structural Theory of Organic Chemistry, Prentice–Hall, 1969.
4. Gould E.S., Mechanism and Structure in Organic Chemistry, Henry Holt and Co., New York, 1959.
5. Jerry March, Advanced Organic Chemistry, 6th Edition, Wilely, New York, 2002.
6. Lowry T.H., and Richardson K.S., Mechanism and Theory in Organic Chemistry, ELBS, New Delhi, 1995.
7. Pinc H., Hendrickson J.B., Cram D.J., and Hammond G.S., Organic Chemistry, 4th Edition, McGraw–Hill Kogakusha Ltd., Tokyo, 1980.
8. Shorter J., Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford, 1973.
9. Sykes P., Guide Book to Mechanism in Organic Chemistry, 6th edn, Pearson, 2002.

♣♣♣♣♣♣♣♣♣♣

I YEAR – I SEMESTER
COURSE CODE: 7MCH1C2

CORE COURSE-II–INORGANIC CHEMISTRY–I

Objectives:

- To enable the learners to understand the Ionic bonding, bond properties.
- To know Acid-base systems and non-aqueous solvents, bonding applications.
- To understand the basic concepts of main group elements, and solid state chemistry.

Unit I: Chemical Periodicity [15 hrs]

Ionic radii – covalent radii – Vander Waals Radius – bond length, bond order, bond energy, bond polarity – partial ionic character of covalent bonds – electro negativity – electron affinity – Lattice energy – Born-Lande equation-Born Haber cycle – Covalent character in ionic compounds – Fajan's rule - different types of electrostatic interactions – hydrogen bonding. Calculation of ionic radius – Pauling's method and Linde's method. Effective nuclear charge – Slater's rule.

Unit II: Nature of chemical bonding [15 hrs]

Valence bond theory – hybridisation – quantum mechanical treatment for sp, sp^2, sp^3 hybridisation – Molecular orbital theory – MO theories to the structure of homonuclear (H_2, B_2, C_2, N_2) and heteronuclear (CO, NO, HCl, HF) diatomic and selective polyatomic molecules (CO_3^{2-}, NO_2, BeH_2, CO_2), comparison of VB and MO theories. VSEPR theory and its applications to H_2O, NH_3, IF_5, IF_7, ClO_4^- ions, like Xenon halides and xenon oxides.

Unit III: Acid-base systems and non-aqueous solvents [15 hrs]

A generalized acid base concepts – steric effects and solvation effects – Measures of Acid – Base strength –Factors affecting the strength of acids and bases – common ion effect and Henderson's equation – Hard and Soft acids and bases – symbiosis – theoretical basis of hardness and softness.

Classification of solvents – properties of ionizing solvents. Typical reactions in non – aqueous solvents – liquid HF, Hydrogen cyanide, Sulphuric acid and acetic acid.

Unit IV: Main Group Chemistry [15 hrs]

Chemistry of borazines and boron nitrides – chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes and silicon nitrides.

P-N compounds, cyclophosphazanes and cyclophosphazenes – S-N compounds – S_2N_2, S_4N_4, (SN)x, polythiazyl S_xN_4 compounds, S-P compounds – molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}.

Unit V: Solid state chemistry **[15 hrs]**

Defects in crystal – different types of defects – line and plane defects – stoichiometry and non- stoichiometry defects and effects of defects on physical properties – types of solids – electronic structure of solids – free electron and band theories. Electrical conductivity and superconductivity – High temperature superconductivity – types of Semi-conductors - semiconductors in solar energy conversion.

Books for Refernce:

1. H.J.Emelius and Sharpe, Modern aspects of Inorganic chemistry, Universal Book Stall, New Delhi, 1989.
2. J.E.Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry – Principles of structure and reactivity, 4th edition, Pearson – Education, 2002.
3. F.Basolo and R.G.Pearson, Mechanism of Inorganic Reactions, Wiley Eastern, 1967.
4. K.F.Purcell and J.C Koltz, An Introduction to Inorganic Chemistry W.B. Saunders Company, Philadelphia, 1980.
5. P.W.Atkins, D.KShriver and C.H.Langfood, Inorganic Chemistry oxford – ELBS**,** U.K 2009.
6. H.V. Keer, Principles of the Solid State, Wiley Eastern Ltd., 1993.
7. B.R.Puri and L.R.Sharma and K.C.Kalia, Principles of Inorganic Chemistry, Milestone Publishers,New Delhi 2008.
8. G.S.Manku, Inorganic Chemistry, TMH Co., 1984.
9. F.A Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edn, John Wiley & Sons Singapore 1998.
10. O.H. Mathur and D.P Tandon, Chemistry of rare elements. S. Chand & Co, IV Edn (1986).
11. K.M.Mackay and R.A. Mackay, Introduction to Modern Inorganic Chemistry, 4th Edn, Prentice Hall, New Jersy 1989.
12. M. C. Day, J. Selbin and H. H. Sisler, Theoretical Inorganic Chemistry; Literary Licensing (LLC), Montana, 2012.
13. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th Ed., A Wiley - Interscience Publications, John Wiley and Sons, USA, 1999.
14. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row publisher, Singapore, 2006

♣♣♣♣♣♣♣♣♣

I YEAR – I SEMESTER
COURSE CODE: 7MCH1C3

CORE COURSE-III–PHYSICAL CHEMISTRY–I

Objectives:

- To enable the learners to understand the significance of electrochemistry
- To know the details of phase rule, thermodynamics and surface chemistry.

Unit I: Electrolytic conductance and Electro kinetics [15 Hrs]

Theory of electrolytic conductance – ionic activity and activity coefficient – Ionic strength – Debye – Huckel theory – Limiting Law – Ionic association – Molar conductivity – Debye – Huckel – Onsager equation – Applications of conductivity measurement – Electrode potential – Helmholtz electrical double layer – Standard electrode potentials – Nernst equation – Applications of Nernst equation – Electrochemical cells and their types – Applications of cell EMF measurements (G, S and H calculations). Calculation of equilibrium constants and solubility products – Over voltage – Hydrogen overvoltage – Butler -Volmer equation, Tafel equation.

Unit II: Classical Thermodynamics [15 Hrs]

Terminology in thermodynanics – I-law of Thermodynamics – limitations – Need for Second law of thermodynamics – Second law of thermodynamics Statements – concept of entropy – Gibbs and Helmhotz free energy – Spontaneity – Gibbs-Helmholtz equation – Van't Hoff Isotherm – Partial molar quantities, partial molar volume – chemical potential, Gibbs -Duhem equation – Experimental determinations of fugacity of real gases and its determination – activity and activity co-efficient – determination.

Unit III: Chemical and Phase Equilibria [15 Hrs]

Chemical Equilibria: Spontaneous reaction – Free energy change for Spontaneous reaction – Significance – Law of mass action, Equilibrium Constant – Van't Hoff equations – Types of equilibrium – Le-Chatelier's Principle – Factors affecting chemical equilibrium.

Phase Equilibria: Gibbs Phase rule – Derivations of Gibb's Phase rule – Two component systems (KI-H_2O system, $FeCl_3$-H_2O system, Zinc-Magnesium System, Sodium sulphate and water system)

Unit IV: Statistical Thermodynamics [15 Hrs]

Aims of statistical thermodynamics – thermodynamic probability – probability theorem – definitions of state of a system – ensembles (micro, macro and grand canonical) – Boltzmann distribution law and its derivations – Boltzmann-Planck equation – Partition functions – thermodynamic properties from partition functions – partition function and equilibrium constant – Quantum statistics – Fermi-Dirac and Bose-Einstein statistics – population inversion.

Unit V: Colloids and Surface Chemistry [15 Hrs]

Colloids: Classification of Colloids – Sols, Lyophilic and lyophobic sols, properties of sols, coagulation. Electrical properties of colloids – Charge on colloidal particles – Electrical double layer – Zeta potential – Electro kinetic properties – Electrophoresis – Electro osmosis.

Surface Chemistry: Introduction – adsorption of gases on solids – physisorption and chemisorptions – adsorption isotherms – Freundlich – Langmuir – BET – Temkin adsorption isotherms – adsorption on liquid surface – surface tension – Gibbs adsorption isotherm – surface area determination by electro-osmosis and electrophoresis.

Books for Reference:

1. J.Rajaram and J.C.Kuriakose, Thermodynamics (III Edn.) shoban Lai Nagin, Chand & Co., New Delhi (1999).
2. D.Attwood and A.T.Florence, surfactant systems – Their chemistry, Pharmacy and Biology, Chapmann and Hall, New-York (1983).
3. S.Glasstone, Thermodynamics for chemists, East – West Press private Ltd., New Delhi.
4. Gurdeep Raj, Advance Physical chemistry (25^{th} Edn.,) Goel Publishing Co., Publishing Co.,(2001).
5. D.A.Mc Quarrie and J.D.Simon, Physical chemistry. A molecular Approach, Viva Books (p) Ltd., New Delhi (1998).
6. P.W.Atkins, physical chemistry. VI, Edn., ELPS and Oxford University Press (1996).
7. A.W.Adamson, Physical Chemistry of Surfaces, 5^{th} Edn., John Wiley & Sons, New York, (1990).
8. L.Antropov. Theoretical electrochemistry MIR Publication Moscow 1972.
9. A.W.Adamson, physical chemistry of surfaces, 5^{th} Edn., John Wiley & sons, New York (1990).
10. B.R.Puri, L.R.Sharma and M.S.Pathania, Principles of Physical chemistry (Millennium Edn,) Vishal Publishing Co., (2003).
11. D.N.Bajpai, Advanced physical chemistry, S.Chand & Company Ltd, New Delhi (1998).
12. J.O.M. Bockris and A.K.N. Reddy, Electrochemistry, Vols. 1 and 2, Plenum, New York 1977.
13. C.M.A.Brett and A.M.O.Brett, Electrochemistry, Principles, Methods and application, OUP, Oxford (1993)

♣♣♣♣♣♣♣♣♣

I YEAR – I SEMESTER
COURSE CODE: 7MCH1P1

CORE COURSE-IV–INORGANIC PRACTICAL–I

Objectives:

- To enable the learners to apply the principle in the semi-micro analysis of an inorganic salt mixture.
- To prepare the inorganic complexes.

1. Semi – micro qualitative analysis: Analysis of mixtures containing one familiar and one less familiar cations from the following W, Pb, Se, Te, Mo, Cu, Cd, As, Sb, Ce, Th, Zr, Ti, V, Cr, Mn, U, Ni, Co, Zn, Ca, Ba, Sr, Li, Mr (insoluble and interfering anion may be avoided).

2. Estimation of one metal ion in the presence of another by EDTA.

3. Inorganic preparations: preparation of at least 5 inorganic complexes.

Books for Reference:

1. J. Bassett *et al*, Text Book of Quantitative Chemical Analysis", 5th Edition, ELBS, Longmann, U.K., 1989.
2. V.V. Ramanujam, "Inorganic Semimicro Qualitative Analysis", The National Publishing Co, Chennai 1974.

♣♣♣♣♣♣♣♣♣

I YEAR – I SEMESTER
COURSE CODE: 7MCH1E2

ELECTIVE COURSE-I (B)–POLYMER CHEMISTRY

Objectives:

- To enable the learners to understand the chemistry of polymers, kinetic mechanism and their degradation.

Unit I: Classification of Polymers and Chemistry of Polymerisation [15 Hrs]

Classification of Polymers, linear polymers, non-linear or branched polymers, cross – linked polymers, homo chain, hetero chain, homopolymers co-polymers, block polymers and graft polymers. Degree of polymerization: Types of polymerization – mechanism of Addition polymerisation – (Free radical, ionic and co-ordination mechanism) – Rubber and Vulcanisation of Rubber.

Unit II: Individual Polymers [15 Hrs]

Individual Polymers: Preparation, properties and applications of polystyrene, polyacrylonitrile, polymethylmethacrylate, Polytetrafluoroethylene, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethylene, phenol – formaldehyde, urea – formaldehyde, melamine – formaldehyde and epoxy resins.

Unit III: Properties of Polymers [15 Hrs]

Intrinsic properties – processing properties – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotatic, isotatic and atatic polymers.

Glass transition temperature: Definition – factors affecting glass transition temperature – relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer.

Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights – molecular weights and degree of polymerization – poly-dispersity – molecular weight distribution in polymers – size of polymer molecules – kinetics of polymerization.

Unit IV: Polymerisation Techniques and Degradation of Polymers [15 Hrs]

Polymerisation Techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations, Degradation: Types of degradation – thermal, mechanical, ultrasonic and photo degradation – photo stabilizers – oxidative degradation – antioxidants – hydrolytic degradation.

Unit V: Polymer Processing **[15 Hrs]**

Compounding of plastics, Rubber and fibres – (plasticizers, colorants, flame retardants) - Polymer processing - Compression, blow and injection mouldings – film extrusion and calendaring – die casting and rotational casting – thermo foaming – reinforcing. Biopolymers – Biomedical polymers – Contact lens, Dental polymers, Artificial Heart, Kidney, Skin and Blood cells.

Books for Reference:

1. V.R.Gowarikar, N.V. Viswanathan and Jayadev Sreedher, "Polymer Science", Wiley Eastern Ltd., New Delhi, 2001.
2. B.K.Sharma, "Polymer Chemistry", Goel Pub., House, Meerut, 2009.
3. F.W.Billmeyer, "Text Book of Polymer Science", 3rd edn., John Wiley and sons, New York, 2004.
4. P.Bahadur, N.V.Sastry, Principles of Polymer Science, II nd Edn., Narosa Pub. House Pvt. Ltd., New Delhi, 2005.
5. G.S.Mistra, Introductory Polymer Chemistry, New Age International Pub., New Delhi, 2005.

♣♣♣♣♣♣♣♣♣♣

II YEAR – III SEMESTER
COURSE CODE: 7MCH3C1

CORE COURSE-IX–ORGANIC CHEMISTRY–III

Objectives:

- To have a knowledge of Molecular rearrangement and addition reactions.
- To know the details of terpenes, Organic Photo chemistry.
- To know about synthetic methods.

Unit I: Reactions and Rearrangements [15 Hrs]

Mechanism of the following rearrangements: Wagner-Meerwin, Dienone-phenol rearrangement, Demjanov, Curtius, Wolff, Baeyer -Villiger, Stevens, Favorski, Cope, Fries and Di–pi methane rearrangement. Mechanism of sommelet reaction – vilsmeir haak reaction – Arndt-Eistert reaction.

Unit II: Addition to multiple bond [15 Hrs]

Electrophilic, Nucleophilic and free radical additions – Addition to Conjugated Systems – Orientation of the addendum – Sharpless asymmetric epoxidation, Addition to α, β – unsaturated Carbonyl groups.

Michael addition – Addition of Grignard reagent to α, β – unsaturated carbonyl groups. Diels- Alder reaction – Addition of Carbenes and Carbenoids to double and triple bonds.

Addition to Carbonyl Group: Mechanism of Mannich reaction, Claisen ester condensation, Darzen's reaction, Reformatsky reaction, wittig reaction and Shapiro reaction.

Unit III: Terpenoids [15 Hrs]

Terpenoids: Classification of terpenoids, structure, and synthesis of α–pinene, Camphor, Zingiberene, Cadinene and abietic acid – Biosynthesis of terpenoids.

Unit IV: Synthetic Methods [15 Hrs]

Planning a synthesis – relay approach and convergent approach to total synthesis – Retro synthetic analysis of simple organic compounds – Functional group interconversions – use of activation and blocking groups in synthesis – Homogeneous hydrogenation – Umpolung synthesis – Robinson annelation – A schematic analysis of total synthesis of the following compounds: 2, 4 – dimethyl-2-hydroxypentanoic acid, Trans-9-methyl-1-decalone.

Unit V: Organic Photochemistry [15 Hrs]

Thermal Vs Photochemical reactions – Allowed and forbidden transitions – Fluorescence – Internal conversion – Intersystem crossing – Jablonski diagram.

Photochemical reactions of Ketones – photosensitization – Norrish type I and Norrish type –II reactions – Paterno - Buchi reaction – Photo oxidation – photo reduction.

Pericyclic reactions: conservation of orbital symmetry – Electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangements – applications of correlation approach, Frontier Molecular orbital approach.

Books for Reference:

1. DeMayo P., Molecular Rearrangements, Academic Press, London.
2. Gould E.S., Mechanisms and Structure in Organic Chemistry, Henry Holt and Co., New York, 1959.
3. Harris J.M., and Wamser C.C., Fundamentals of Organic Reaction Mechanisms, John Wiley and Sons Inc., New York, 1976.
4. Mukerji S.M., and Singh S.P., Reaction Mechanisms in Organic Chemistry, McMilan India Ltd, 1978
5. Agarwal O.P., Natural Products, Vol. I and II, Goel Publication, Meerut.
6. De Mayo P., Chemistry of Terpenoids, Vol. I and II, Academic Press, London.
7. Morrison R.T., and Boyd R.N., Organic Chemistry, Prentice – Hall, 6th Edition, New Delhi, 1995.
8. Bellamy A.J., An introduction to Conversation of Orbital Symmetry, Longman, England, 1974.
9. Depuy C.H., and Chapman O.L., Molecular Reactions and Photo Chemistry, Prentice – Hall, New Delhi, 1972.
10. Finar I.L., Organic Chemistry Vol.–II., ELBS, England, 1975.
11. Ireland R.E., Organic Synthesis, Prentice – Hall of India (P) Ltd, New Delhi, 1975.
12. March J., Advanced Organic Chemistry, Wiley, 6th Edition, New York, 2007.

♣♣♣♣♣♣♣♣♣♣

II YEAR – III SEMESTER
COURSE CODE: 7MCH3C2

CORE COURSE-X–INORGANIC CHEMISTRY–III

Objectives:

- ✍ To enable the students in-depth study of spectral applications to the structural elucidation of inorganic compounds.
- ✍ To know the details *of* lanthanides and actinides.
- ✍ To understand the concept of cages and metal clusters.

Unit I: Application of IR, Raman and Mossbauer Spectroscopy to the Study of Inorganic Compounds [15 hrs]

Application of IR and Raman spectra in the study of coordination compounds – application to metal carbonyls, nitrosyls and sulphate – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding.

Mossbauer Spectroscopy: Mossbauer Effect – resonance absorption – Doppler effect – Doppler velocity – isomer shift –magnetic hyperfine splitting-application of Mossbauer spectroscopy in the study of iron and tin complexes.

.

Unit II: Electronic Spectra and NMR Spectroscopy of Inorganic Compounds [15 hrs]

d-d transition – charge transfer transition – selection rules – mechanism of beak down of selection rules – bandwidths and shapes – Jahn Teller effect – Orgel diagram - evaluation of 10Dq and β for octahedral and tetrahedral complexes.

NMR Spectroscopy: ^{31}P and ^{19}F and – NMR spectroscopy – Introduction – application in structural problem – evaluation of rate constants – monitoring the course of reaction – NMR of fluxional molecules – NMR of paramagnetic molecules – contact shifts and shift reagents.

Unit III: Metallurgy and Complexes [15 hrs]

Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Pb and Se.

Complexes of π- acceptor ligands: Synthesis, properties, structure and bonding in mononuclear and dinuclear metal carbonyls – Application of EAN rule. Synthesis, properties, structure and bonding in Ferrocene complexes – magnetic properties.

Unit IV: Lanthanides and Actinides [15 hrs]

Lanthanides: Occurrence – separation techniques (precipitation, ion-exchange, solvent-extraction and Selective reduction and oxidation) – Electronic configuration – Oxidation states, Lanthanide contraction – Spectral and Magnetic properties- Lanthanides as shift reagents in NMR – uses of lanthanides and their compounds – position in the periodic table.

Actinides: Synthesis of elements – Extraction of Th, U and Pu from fission products-electronic configuration and oxidation states, spectral and magnetic properties – position in the periodic table.

Unit V: Cages and metal clusters **[15 hrs]**

Electron deficient compounds: Borane and carboranes – nomenclature – Synthesis, properties, structure and bonding in diborane and tetraborane – wades rule – Styx numbers.– Synthesis, properties and structure of Ferrocene.

Metal clusters: Polyacids – classification of polyacids – synthesis, structure and bonding in poly anions and isopoly anions of phosphorous, Molybdenum and tungsten.

Books for Reference:

1. F.Basalo and R.G. Pearson, Mechanism of Inorganic Reactions, 2nd End., Wiley New York, 1973
2. R.S Drago, Physical Methods in Chemistry, Saunder Golden Sunburst Series, W.B. Saunders company; London 1977.
3. Raymond Chang- Basic principles of Spectroscopy, Mc Graw Hill,New Delhi. 1971.
4. Nakamoto, Kazuo, Infrared and Raman Spectra of Inorganic and coordination compounds, IV edition, John Wiley and Sons,New Yark,1986.
5. J.D.Woolings, Non Metal Rings, Cages and Clusters, John Wiley and sons, New York, 1989.
6. R. S. Drago, Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
7. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 2011.
8. Wahid U.Malik, G.D. Tuli and R.D.Madan, Selected Topics in Inorganic Chemistry, S.Chand & Co. Ltd., New Delhi, 2006.
9. Douglas and McDaniel, A Concise of Inorganic Chemistry, - Oxford and IBH Publishing company (P)Ltd., New Delhi. 2002.
10. E. Huheey, Ellen A.Keiter, Richard L.Keiter, Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
11. William W. Porterfield, Inorganic Chemistry, Elsevier, II Edn., New Delhi.2005.
12. A.G. Sharpe, Inorganic Chemistry, Addition – Wesley Longman, UK III Edn., 2004.
13. Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn.,New Delhi. 2004.
14. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, Universities Press (India) Limited, 2001.

♣♣♣♣♣♣♣♣♣

II YEAR – III SEMESTER
COURSE CODE: 7MCH3C3

CORE COURSE-XI–PHYSICAL CHEMISTRY–III

Objectives:

- To understand the principles of quantum chemistry and Macromolecules.
- To enable the learners to acquire knowledge in catalysis.

Unit I: Photo and Radiation Chemistry [15 Hrs]

Physical properties of the electronically excited molecules – Photophysical Process – Jablonski's diagram – radiationless transitions – Internal conversion and intersystem crossing – Stern-Volmer equation and its application – radiative transition – fluorescence, phosphorescence and other deactivation processes. Effect of temperature on emission process – photosensitization and Chemiluminescence – elementary aspects of photosynthesis – photochemical conversion and storage of solar energy – Experimental techniques in photochemistry – Chemical actinometers. Photochemical Kinetics of H_2-X_2 reactions.

Unit II: Quantum Mechanics – I [15 Hrs]

Planck's explanation about black-body radiation – de-Broglie's concept of matter waves, Compton effect – Heisenberg's uncertainty principle and complementarily. Operators – Linear operators – Method of getting the following quantum mechanical operators – position, momentum, Kinetic energy, potential energy, total energy, angular momentum and spin angular momentum. Postulates of quantum mechanics – Hermicity and proving the quantum mechanical operators are Hermitian – Commutators algebra – evaluation of commutators – vanishing and non – vanishing commutators.

Unit III: Quantum Mechanics – II [15 Hrs]

Eigen function and Eigen Value – Expansion theorem – Orthogonality and normalization of wave functions. Derivation of Schrodinger wave equation – application ***of*** SWE to simple systems – free particle moving in one dimensional box – Characteristics of wave function – average momentum of a particle in a box is zero-particle moving in a 3-D box – degeneracy – distortion – particle moving in ring – rigid rotator.

Unit IV: Application of Quantum Mechanics [15 Hrs]

Spherical harmonics – simple harmonic oscillator – Hermite polynomials – radial wave function – radial probability distribution – shapes of various atomic orbitals. Schrodinger equation for Helium atom and other many electron system. Necessity for approximation methods – Variation methods for the Hydrogen atom – Perturbation (first order) method to Helium atom - Slater determinant wave function – secular determinant – HMO π-electron theory of Ethylene and Butadiene.

Unit V: Fast Reactions, Catalysis and Kinetic theory of gas [15 Hrs]

Catalysis: General Characteristics of Catalysis - Homogeneous Catalysis – Acid-Base Catalysis – Enzyme Catalysis – Derivations of Michaelis & Menton Equation – Heterogeneous Catalysis – Surface reactions – Kinetics of Surface reactions.

Fast reactions – flow and relaxation techniques, Temperature Jump and pressure jump method (Pulse method) – Flash photolysis.

Equations of states – Maxwell-Boltzmann distribution law – Principle of equipartition of energy and heat capacity – Rotation, vibrations and translational degree of freedom – Molecular collisions – Mean free path – transport properties – thermal conductivity.

Books for Reference:

1. A.K. Chandra, Introductory Quantum Chemistry, 4th Edn., Tata Mc Graw Hill Publishing Co, New Delhi, (2006).
2. R.K. Prasad, Quantum Chemistry, Revised 3rd Edn , New Age International Publishers, New Delhi (2009).
3. James.E. House, Fundamentals of Quantum Chemistry, 2nd Edn., Elsevier Publishers India Pvt. Ltd, New Delhi (2005).
4. IRA N.Levine Quantum Chemistry, 5th Edn., Prentice – Hall of India Pvt. Ltd, New Delhi (2006).
5. K.K.Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern.
6. P.W. Atkins,Molecular Quantum Mechanics, 5th edn. Oxford University Press, (2012).

♣♣♣♣♣♣♣♣♣♣

II YEAR – III SEMESTER
COURSE CODE: 7MCH3P1

CORE COURSE-XII–PHYSICAL CHEMISTRY PRACTICAL–I

Objectives:

- To know about the practical applications of conductometry, potentiometry and pH metry.
- To get in-depth knowledge in adsorption and kinetic experiments.

I. Conductometric Experiments

i) Double displacement & acid base titration
   a) NH_4C1 – NaOH – Mixture of CH_3COOH & HCl
   b) NH_4C1 – NaOH – Mixture of NH_4C1 & HCl

ii) Precipitation titration
   a) KCl – $AgNO_3$ – KCl
   b) K_2SO_4 – $BaC1_2$ – K_2SO_4

iii) Determination of dissociation constant of weak acids.

iv) Determination of equivalent conductance of weak electrolyte at infinite dilution using Kohlraush law.

II. Adsorption Experiments

Adsorption of Oxalic acid / Acetic and on charcoal.

III. Kinetic Experiments

i) Kinetics of alkaline hydrolysis of ester by conductometric method
ii) Perdisulphate and iodide ion reaction: study of Primary salt effect and determination of concentration of given KNO_3.

IV. Potentiometric methods

i) Precipitation titration: Ag Vs halide mixture
ii) Redox titration: a) permanganate Vs iodide ion b) Ceric ammonium Sulphate Vs ferrous ion
iii) Determination of dissociation constant of weak acids and pH of buffer solutions.
iv) Determination of solubility product of sparingly soluble salts.

V. Titrations using pH meter

Determination of first, second and third dissociation constants of phosphoric acid.

Book for Reference:

1. J.B.Yadav;"Advanced Practical Physical Chemistry"6^{th} Edn.,Goel Publications,Meerut, 1986.

♣♣♣♣♣♣♣♣♣

II YEAR – III SEMESTER
COURSE CODE: 7MCH3E1

ELECTIVE COURSE-III (A)–PHARMACEUTICAL CHEMISTRY

Objectives

- ✍ To enable the learners to know the fundamentals of pharmaceutical Chemistry, concept of chemotherapy and its agents.

Unit I: Introduction to Drug and drug design [15 Hrs]

Historical background-sources and classification of drugs-important terminologies in pharmaceutical chemistry. Concept of drug, lead compound and lead modification, prodrugs and soft drugs.

Structure-activity relationship (SAR) and the development of Quantitative Structure Activity Relationship (QSAR). Factors affecting bioactivity – resonance, inductive effect, isosterism, bio-isosterism, spatial considerations; Theories of drug activity – occupancy theory, rate theory, induced fit theory Concept of drug receptors – elementary treatment of drug-receptor interactions; Physicochemical parameters – lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials;

Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, medicinal chemistry.

Unit II: Antibiotics & Antivirals [15 Hrs]

Structural features and SAR of the following antibiotics – penicillin G, cephalosphorin and their semisynthetic analogs (β – lactam), streptomycin (amino glycoside), terramycin (tetracycline), erythromycin (macrolide) and chloramphenicol. Synthesis of penicillin-V and Chloramphenicol.

Anti-AIDS and Anti-viral agents (A brief study and medicinal importance), Antimalarials - Classification Synthesis of Chloroquine

Unit III: Antineoplastic agents & Psychoactive drugs [15 Hrs]

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Synthesis of antineoplastic agents viz. Mechlorethamine, cyclophosphamide, chlorambucil and 6- mercaptopurine .

Introduction, neutotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, neurochemistry of mental diseases.

Unit IV: Cardiovascular Drugs [15 Hrs]

Cardiovascular Drugs and Local Antiinfective Drugs: Introduction, Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output.

Synthesis of cardiovascular drugs viz. amyl-nitrate, sorbitrate, methyldopa, verapamil and atenolol.

Unit V: Analgesics, anaesthetics and antihypertensive drugs [15 Hrs]

Narcotic analgesics: Analgesic action of Morphine. Synthetic analgesics: pethidine. Non-Narcotic analgesics-aspirin, methyl salicylate, paracetamol and phenacetin

General anaesthetics-Volatile general anaesthetics, Intravenous anaesthetics or non-volatile anaesthetics. Local anaesthetics-Classification.

Synthesis and therapeutic action of Nifedipine, captopril, hydralazine, sodium nitroprusside, clonidine and guanothidine.

Books for Reference:

1. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-HilI **(2005**).
2. S. S. Pandeya & J. R. Dimmock.Introduction to Drug Design, New Age International**.(2000).**
3. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (**2005).**
4. Finar, I. L. & Finar, A. L. Organic Chemistry Vol. 2, Addison-Wesley (1998)
5. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998)
6. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons **(1997).**
7. Patrick, G. L. Introduction to Medicinal Chemistry Oxford University Press (2001).
8. S.S.Pandeya and J.R.Dimmock, An Introduction to Drug Design, New Age, International, 2006.
9. Introductory Medicinal Chemistry, J.B.Taylor and P.D.Kennewell, Ellisworth publishers, 1985.
10. Fundamentals of Medicinal Chemistry by Gareth Thomas, John Wiley & Sons: Chichester, **2003**.
11. Medicinal Chemistry: An Introduction by Gareth Thomas, Wiley-Interscience, 2nd edition, **2008**.
12. An introduction to Medicinal Chemistry by Graham L. Patric, Oxford University Press, USA, 3rd edition, **2005**.
13. Wilson and Giswald's Textbook of Organic Medicinal and Pharmaceutical Chemistry by John Block and John M Beale (Eds), Lippincott Williams & Wilkins, 11th edition, **2003**.
14. The Organic Chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press,2nd edition, **2004**.
15. Jayashree Ghosh, A textbook of Pharmaceutical Chemistry, S.Chand & Company Ltd., New Delhi, 2012.

♣♣♣♣♣♣♣♣♣♣